

# Apocynin

<b>Other names:</b>	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)- Acetophenone, 4'-hydroxy-3'-methoxy- Acetoguaiacon Acetoguaiacone Acetovanillone Acetovanilone Acetovanyllon Apocynine 1-(4-Hydroxy-3-methoxyphenyl)ethanone 3-Methoxy-4-hydroxyacetophenone 4-Acetyl-2-methoxyphenol 4-Hydroxy-3-methoxyacetophenone 4-Hydroxy-3-methoxyphenyl methyl ketone 4'-Hydroxy-3'-methoxyacetophenone 3-Metoksy-4-hidroksyacetofenon 2-Methoxy-4-acetylphenol 3'-Methoxy-4'-hydroxyacetophenone 4-Acetylguaiacol 4-Hydroxy-3-methoxyphenyl methyl keton Phenol, 4-acetyl-2-methoxy NSC 209524 1-(4-Hydroxy-3-methoxyphenyl)-ethanone (acetovanillone) -Acetylguaiacol
<b>Inchi:</b>	InChI=1S/C9H10O3/c1-6(10)7-3-4-8(11)9(5-7)12-2/h3-5,11H,1-2H3
<b>InchiKey:</b>	DFYRUELUNQRZTB-UHFFFAOYSA-N
<b>Formula:</b>	C9H10O3
<b>SMILES:</b>	<chem>COc1cc(C(C)=O)ccc1O</chem>
<b>Mol. weight [g/mol]:</b>	166.17
<b>CAS:</b>	498-02-2

## Physical Properties

Property code	Value	Unit	Source
gf	-260.86	kJ/mol	Joback Method
hf	-426.14	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method

log10ws	-1.80		Crippen Method
logp	1.603		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1498.70		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1490.00		NIST Webbook
ripol	2664.00		NIST Webbook
ripol	2626.00		NIST Webbook
ripol	2637.00		NIST Webbook
ripol	2676.00		NIST Webbook
ripol	2620.00		NIST Webbook
ripol	2620.00		NIST Webbook
ripol	2667.00		NIST Webbook
ripol	2606.00		NIST Webbook
ripol	2664.00		NIST Webbook
ripol	2640.00		NIST Webbook
ripol	2638.00		NIST Webbook
ripol	2640.00		NIST Webbook
ripol	2667.00		NIST Webbook
ripol	2664.00		NIST Webbook
ripol	2640.00		NIST Webbook
ripol	2623.00		NIST Webbook
tb	570.70	K	NIST Webbook
tc	822.63	K	Joback Method
tf	414.01	K	Joback Method
vc	0.421	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.95	J/molxK	593.89	Joback Method
cpg	313.95	J/molxK	632.01	Joback Method
cpg	324.24	J/molxK	670.14	Joback Method
cpg	333.88	J/molxK	708.26	Joback Method
cpg	342.92	J/molxK	746.38	Joback Method
cpg	351.43	J/molxK	784.51	Joback Method
cpg	359.45	J/molxK	822.63	Joback Method
dvisc	0.0007214	Paxs	414.01	Joback Method
dvisc	0.0003744	Paxs	443.99	Joback Method
dvisc	0.0002111	Paxs	473.97	Joback Method
dvisc	0.0001274	Paxs	503.95	Joback Method
dvisc	0.0000814	Paxs	533.93	Joback Method
dvisc	0.0000546	Paxs	563.91	Joback Method
dvisc	0.0000381	Paxs	593.89	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	537.20	K	2.30	NIST Webbook

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Joback Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C498022&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>ripola:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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